

SDBS-¹³C NMR SDBS No. 1716 CDS-12-007
 $C_{13}H_{16}O_2$
4,4'-isopropylidenediphenol

22.53 MHz
0.025 g : 0.5 ml DMSO-d₆

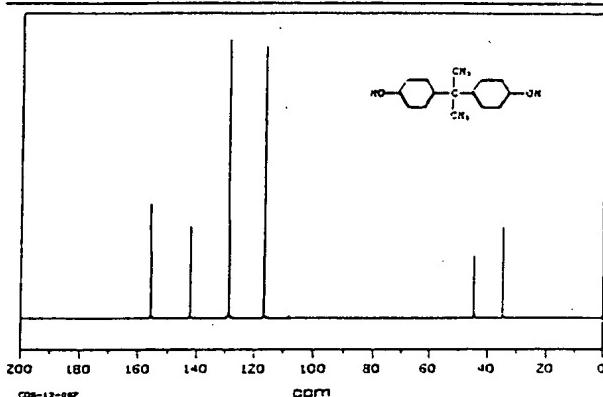
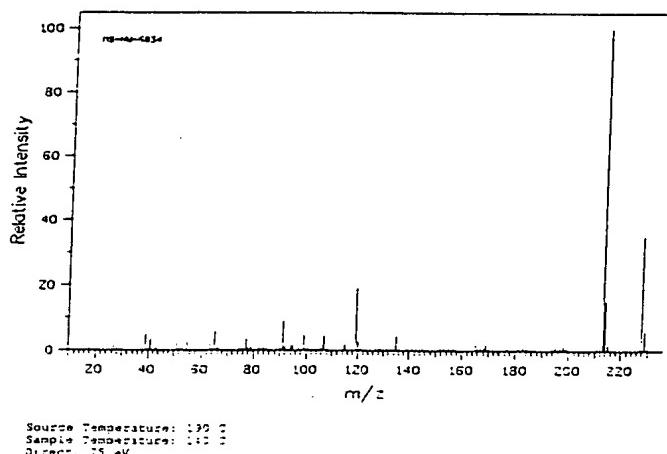


Fig. I (a)

SDBS-Mass

MS-NW-4814 SDBS NO. 1716
4,4'-ISOPROPYLIDENEDIPHENOL
C₁₃H₁₆O₂ Mass >1: molecular ion: 229



HIT-NO-1641 SCORE- 1 SDBS-NO-1716 [R-N10A-05052 : KBR DISC
4,4'-ISOPROPYLIDENEDIPHENOL

C₁₃H₁₆O₂

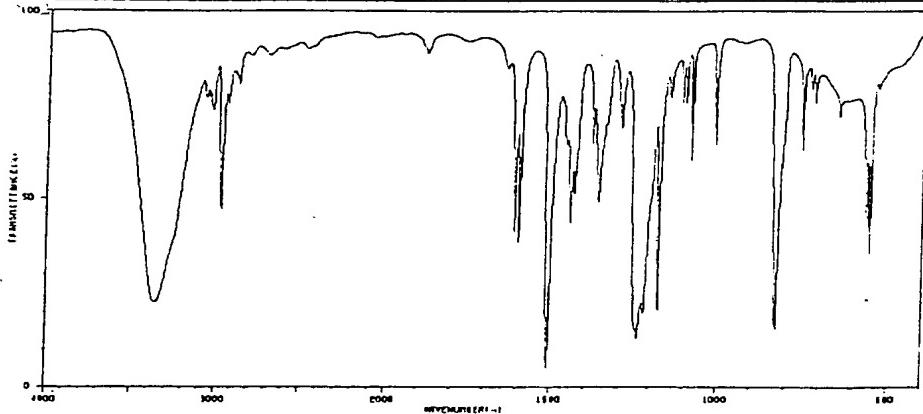
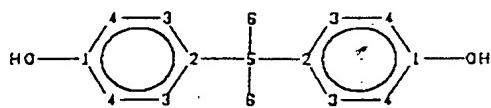


Fig. I (c)



¹³C δ ppm Int. Assign.

154.72	411	1
140.94	330	2
127.11	1000	3
114.43	977	4
40.78	223	5
30.73	323	6

Fig 2(a)

SDRS-Mass

MS-NW-6834 SOBS NO. ~ 1716
 4,4'-ISOPROPYLIDENE DIIPHENOL
 C15H16O2 (Mass of molecular ion: 223)
 m/z ratio

27.0	1
39.0	4
41.0	3
51.0	2
55.0	2
63.0	2
65.0	5
66.0	1
76.0	1
77.0	1
79.0	1
89.0	1
90.0	1
91.0	9
92.0	2
94.0	1
95.0	4
99.0	1
105.0	1
106.5	2
107.0	4
114.0	1
115.0	2
119.0	1
120.0	1
134.0	6
135.0	2
152.0	1
165.0	2
169.0	1
181.0	1
183.0	1
195.0	1
197.0	1
198.0	1
212.0	1
213.0	1
214.0	1
215.0	1
228.2	3
229.0	3

Fig 2(b)

cm^{-1}	%T								
3168	21	2933	72	1436	49	1178	20	816	66
3070	74	2871	77	1384	62	1150	74	759	60
3030	74	1612	39	1303	47	1113	72	735	77
3030	70	1600	37	1296	66	1102	72	724	72
2976	46	1510	4	1247	14	1085	57	650	58
2966	46	1463	62	1239	12	1013	62	565	41
2966	62	1447	42	1221	19	827	14	663	34

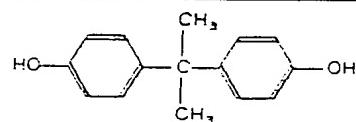
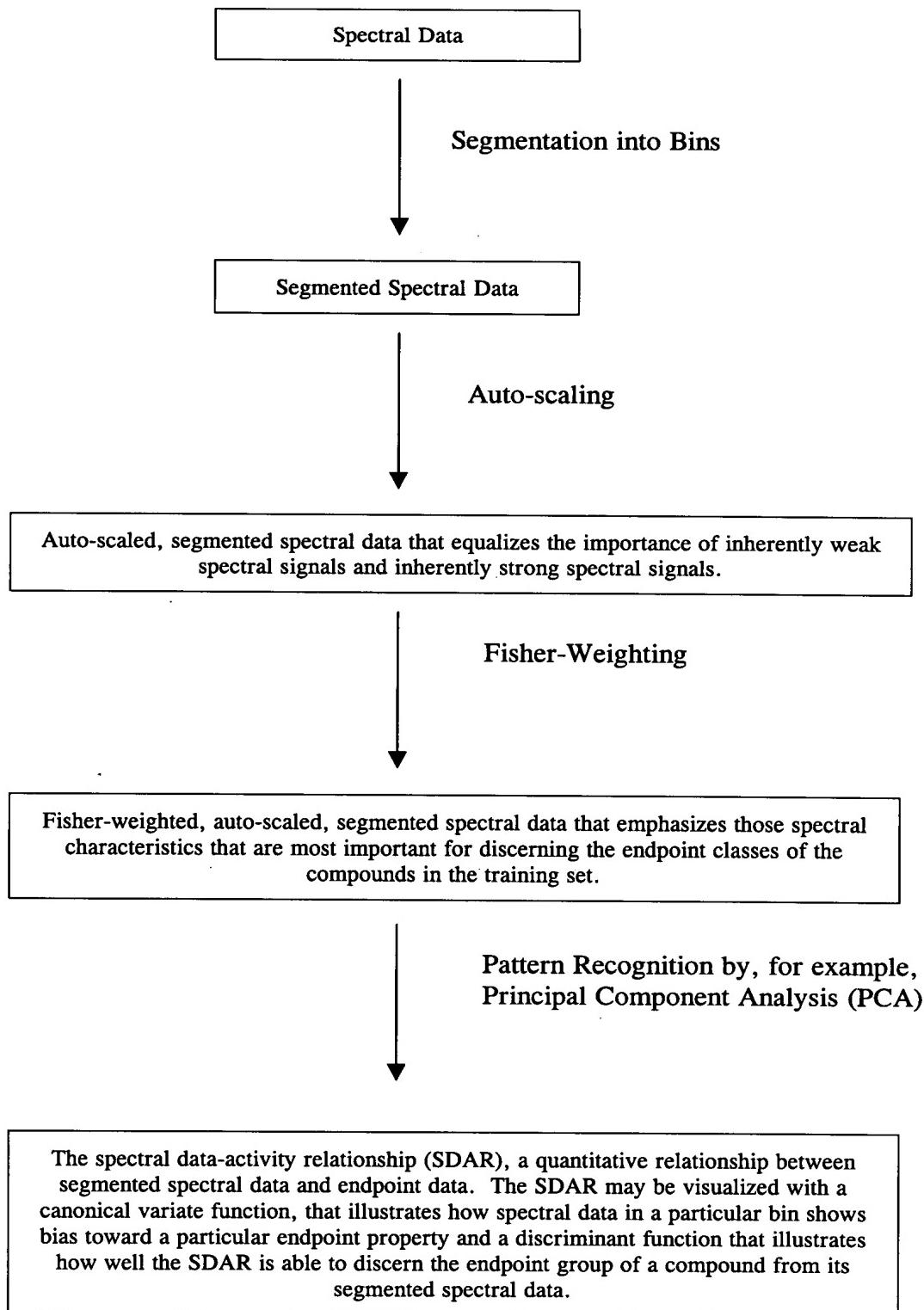


Fig 2(c)

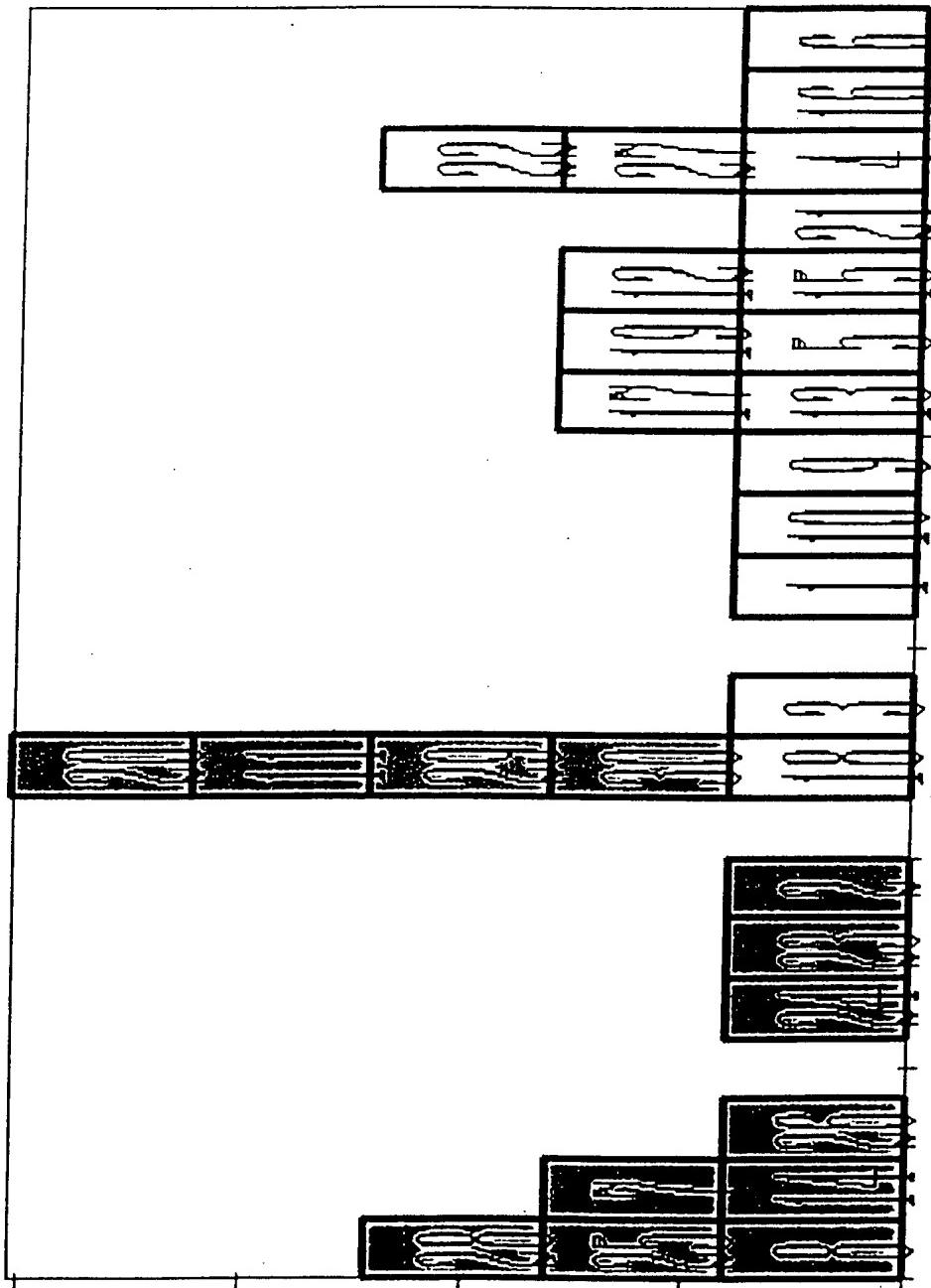
Bin Number	Spectral Intensity	Bin Number	Spectral Intensity	Bin Number	Spectral Intensity
51	2	183	1	1025	62
55	2	195	1	1026	42
63	2	197	1	1027	49
65	5	198	1	1032	62
66	1	212	1	1034	47
76	1	213	100	1041	66
77	3	214	15	1046	14
79	1	215	1	1047	12
89	1	228	35	1048	19
90	1	229	5	1053	20
91	9	580	328	1056	74
92	1	590	223	1059	72
94	2	664	977	1060	72
95	1	677	1000	1062	57
99	4	690	330	1069	62
105	1	704	441	1088	14
106	2	834	21	1089	55
107	4	864	74	1095	60
114	1	866	74	1097	77
115	1	868	70	1098	72
119	19	873	46	1106	68
120	2	874	46	1114	41
134	1	875	62	1115	34
135	4	877	72		
152	1	883	77		
165	2	1009	39		
169	1	1011	37		
181	1	1019	4		

Figure 3 – a hypothetical set of spectrally derived molecular structure descriptors for bisphenol A.

FIG. 4



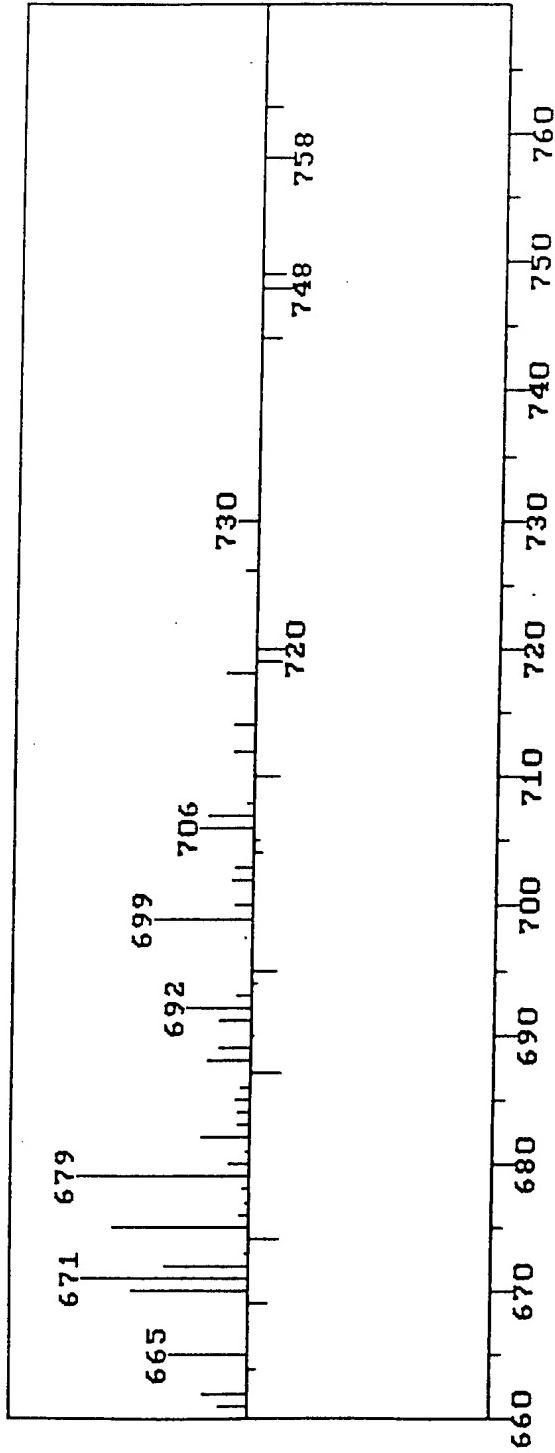
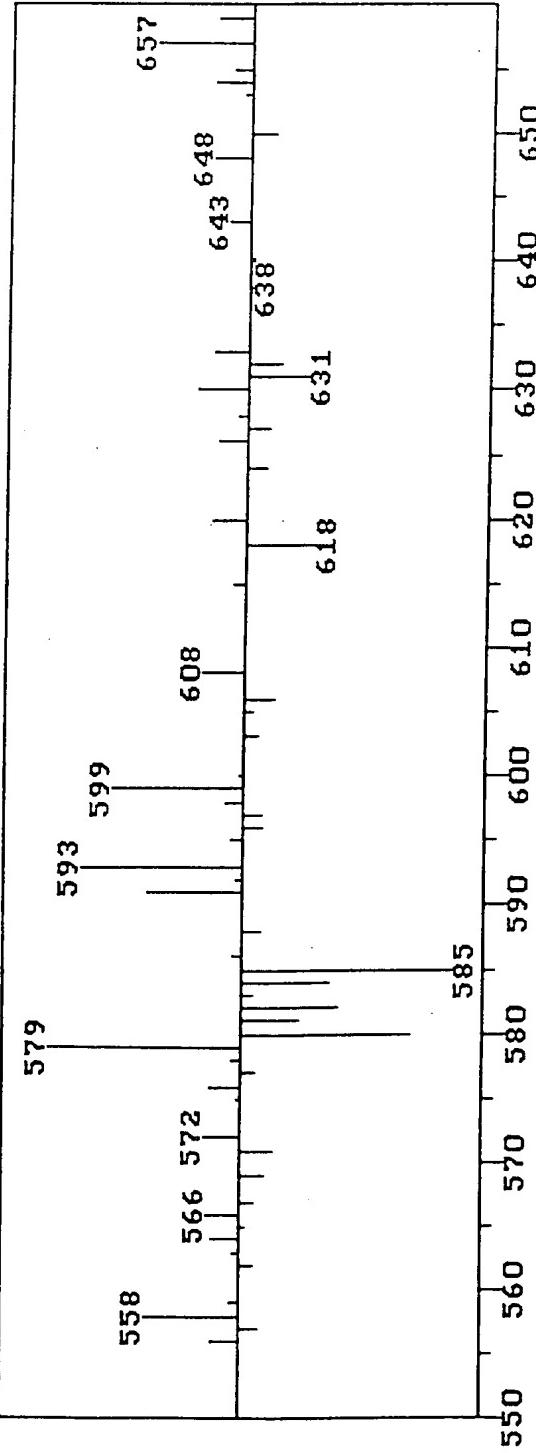
DISCRIMINANT FUNCTION



COMPONENT 1

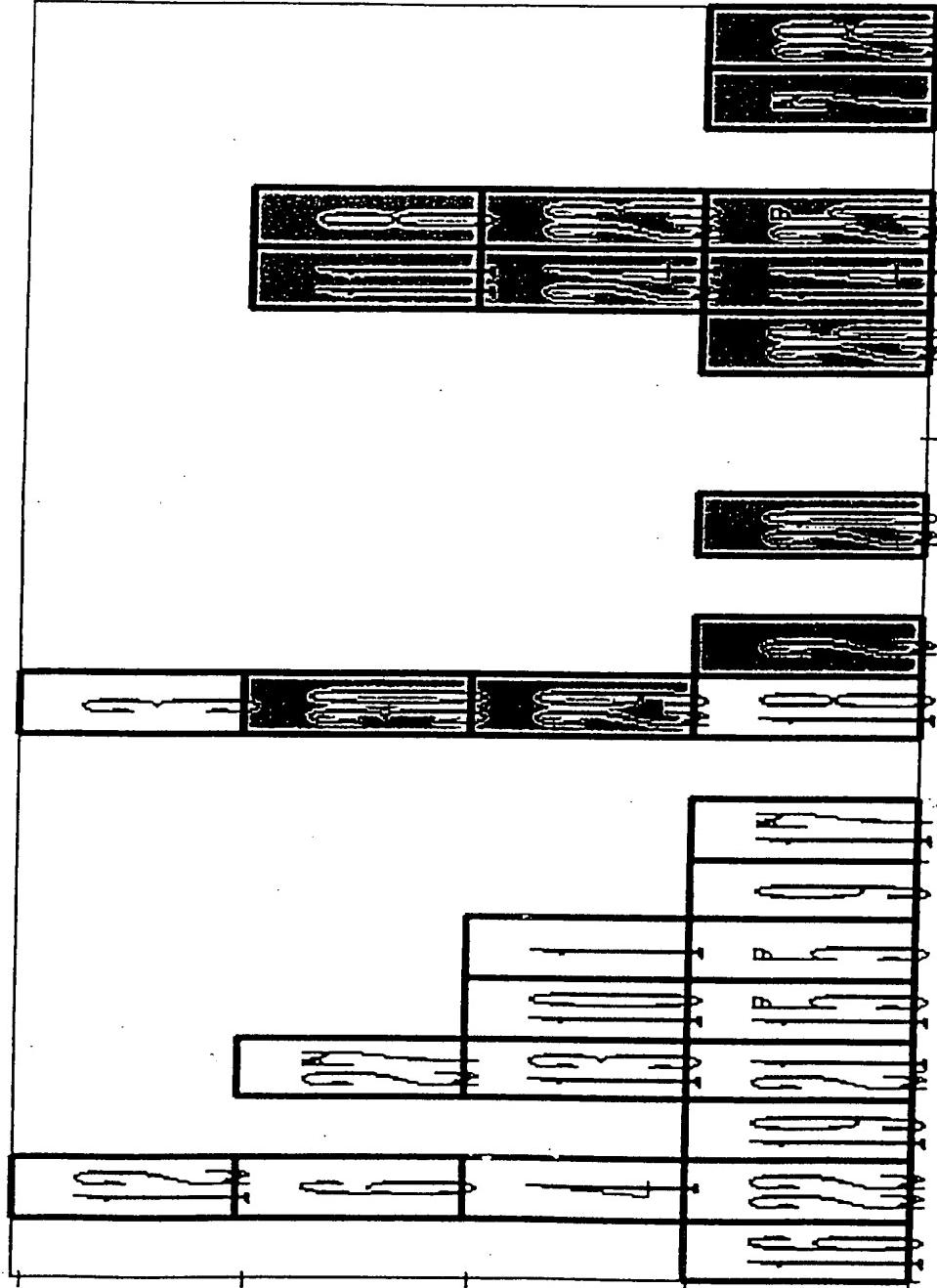
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CANONICAL VARIATE 1



$F/G, G$

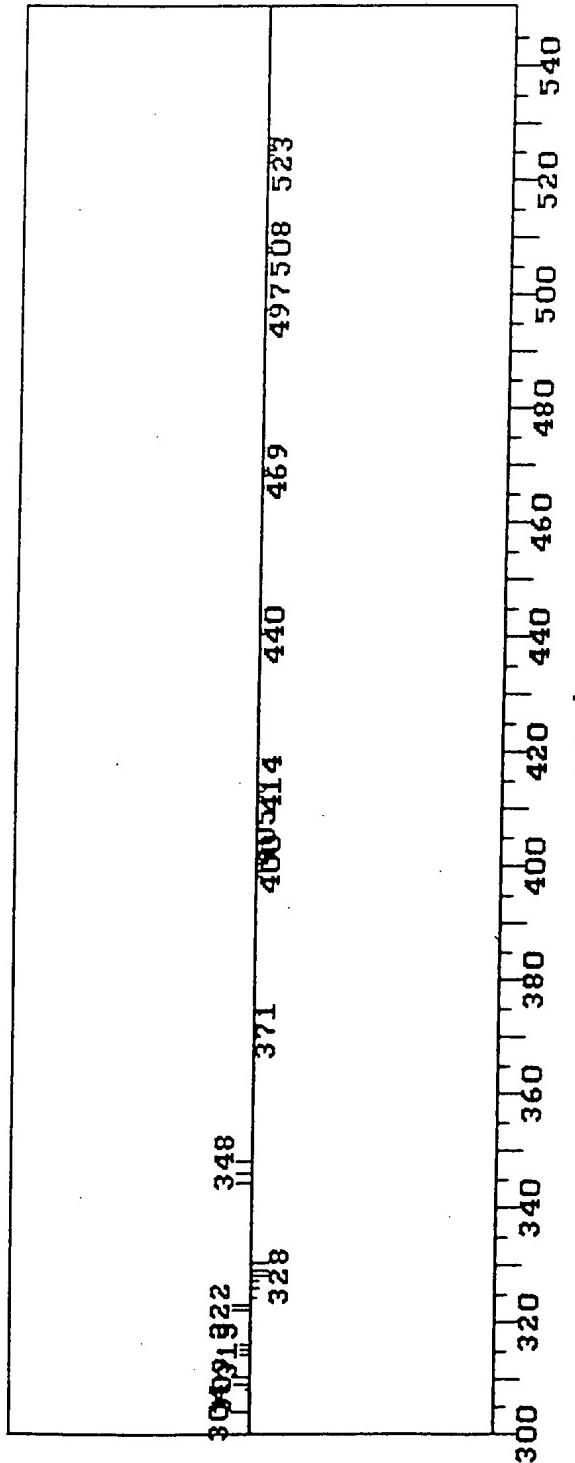
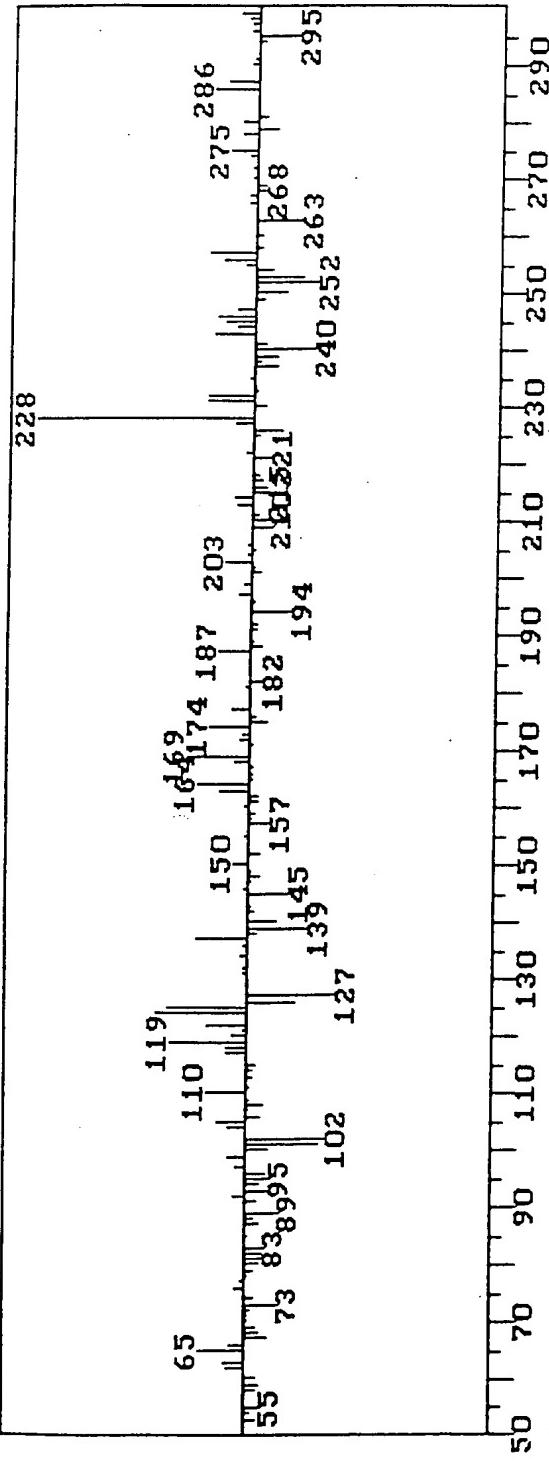
DISCRIMINANT FUNCTION



COMPONENT 1

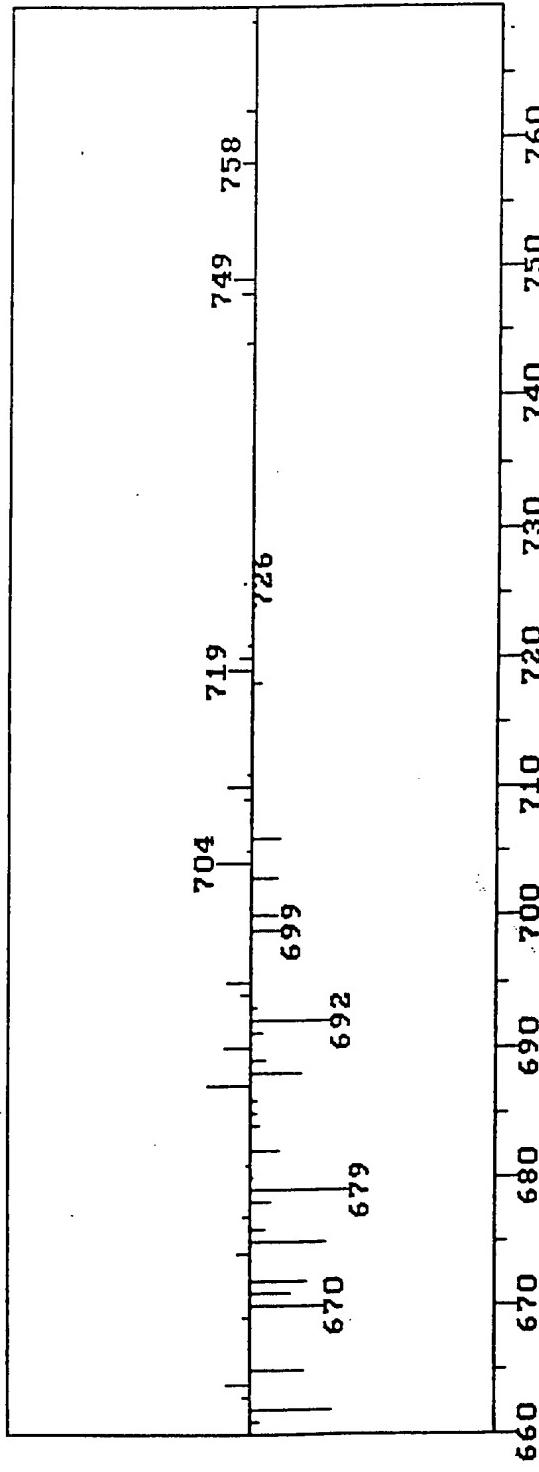
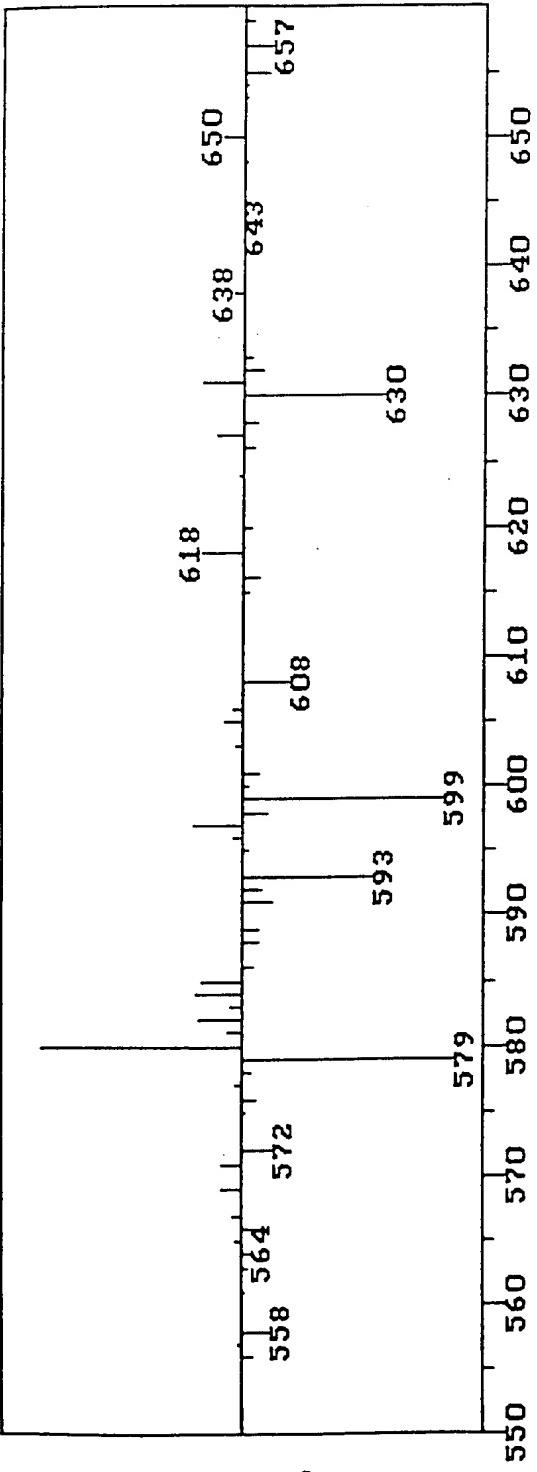
E/G 7
0 2 4 6 8 10 12 14 16 18 20 22 24 26 28 30 32 34 36 38 40 42 44 46 48 50 52 54 56 58 60 62 64 66 68 70 72 74 76 78 80 82 84 86 88 90 92 94 96 98 100

CANONICAL VARIATE 1



$\Sigma G_i S(a)$

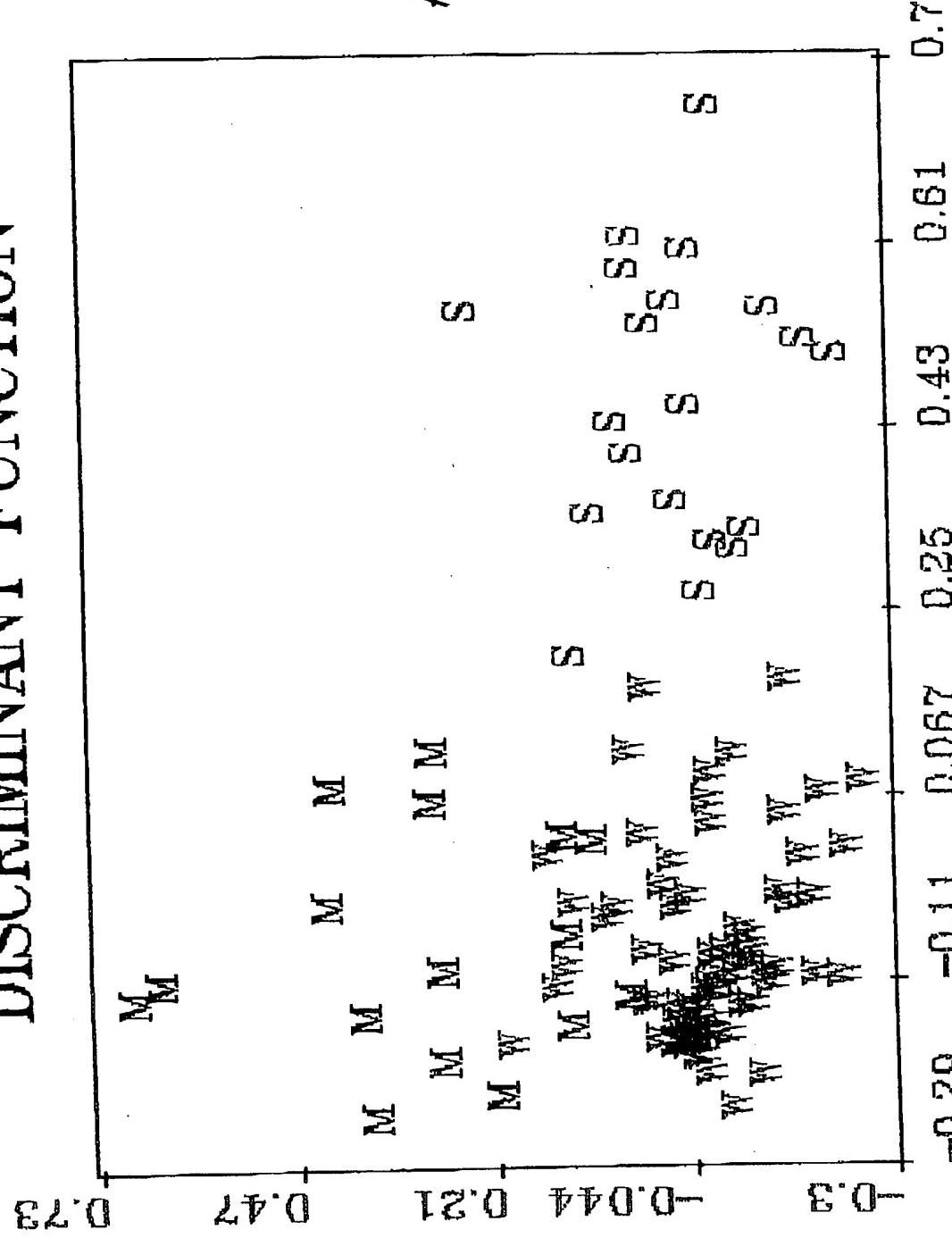
CANONICAL VAPPIATE 1



E. B(6)

DISCRIMINANT FUNCTION

Fig 9



COMPONENT 1

0.29 0.36 0.43 0.50 0.57 0.64 0.71 0.78

CANONICAL VARIATE 1

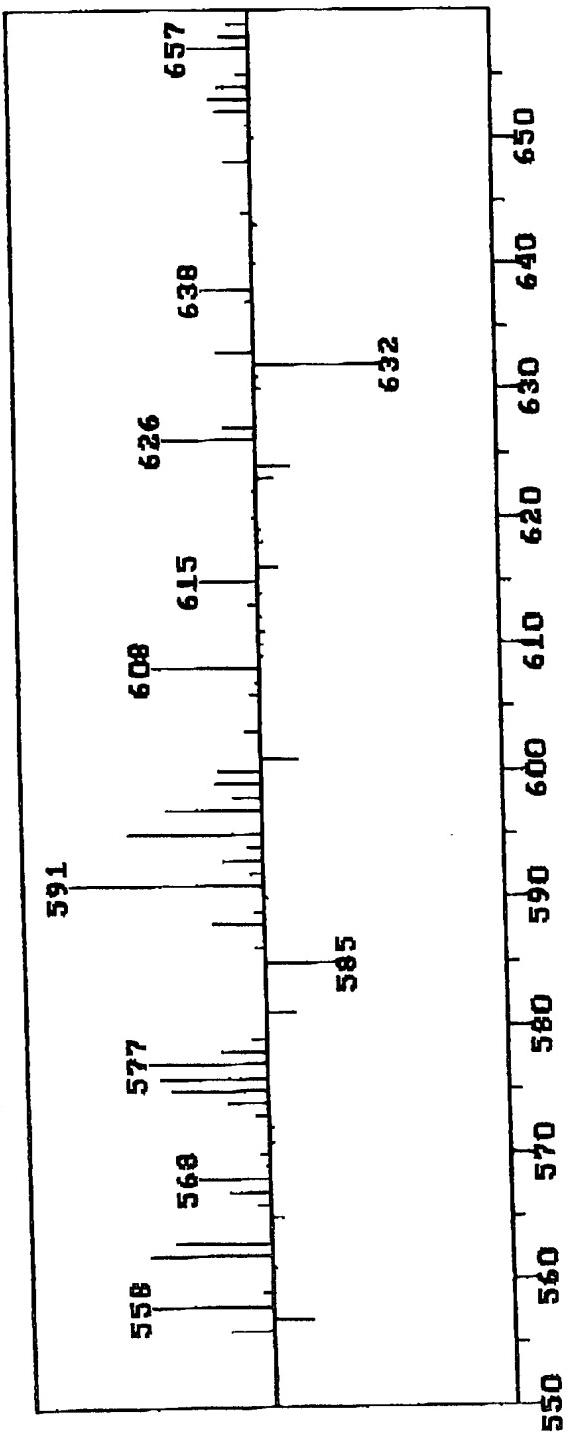
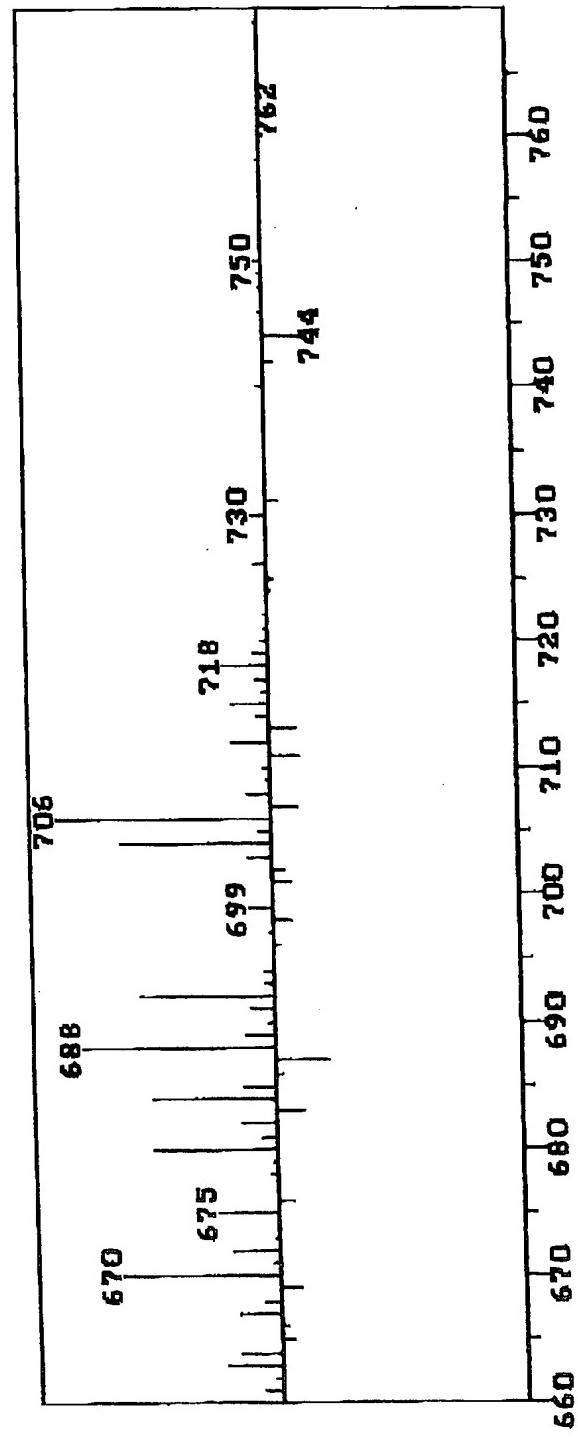
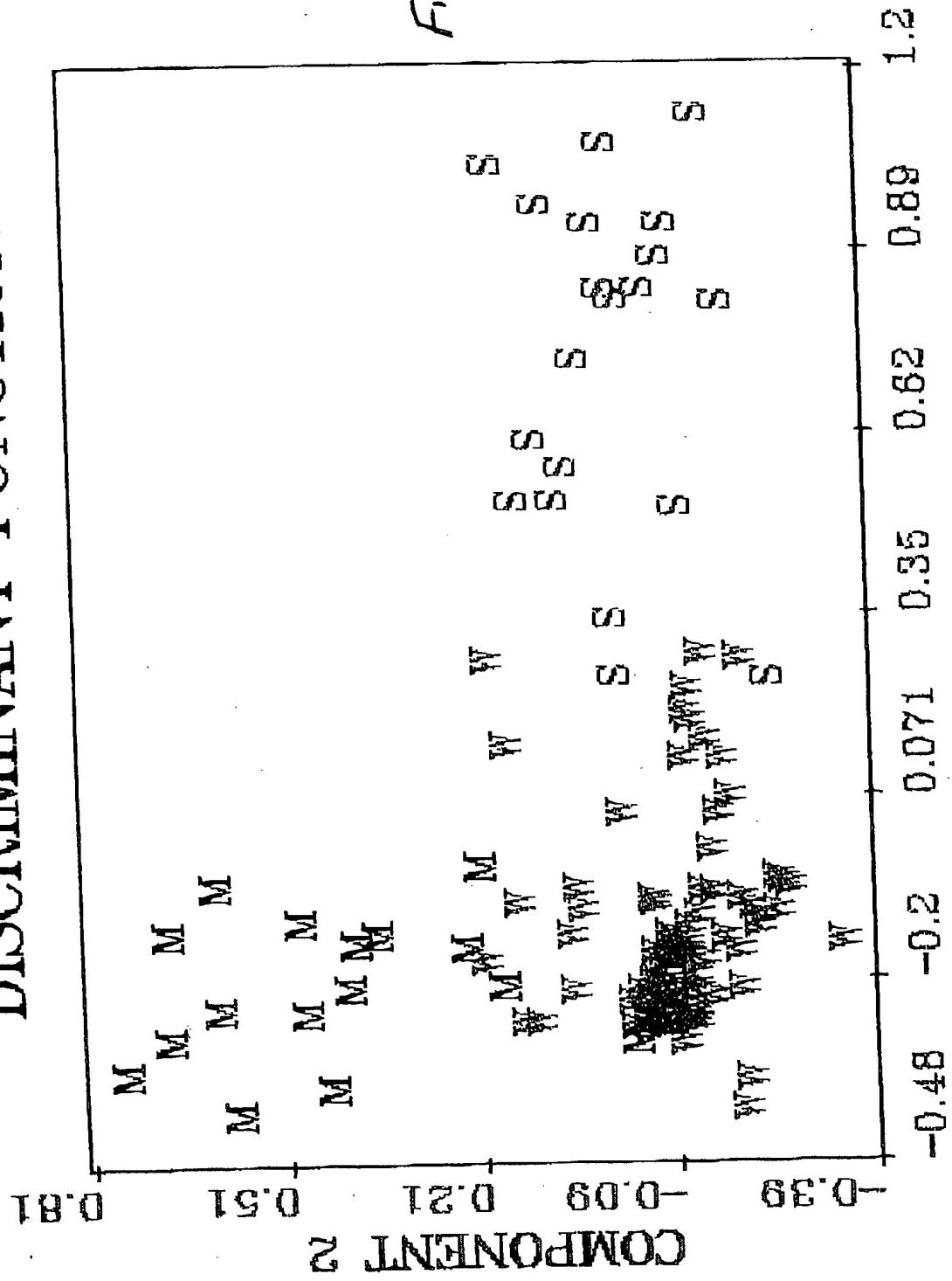


Fig. 10



M/Z

DISCRIMINANT FUNCTION



CANONICAL VARIATE 1

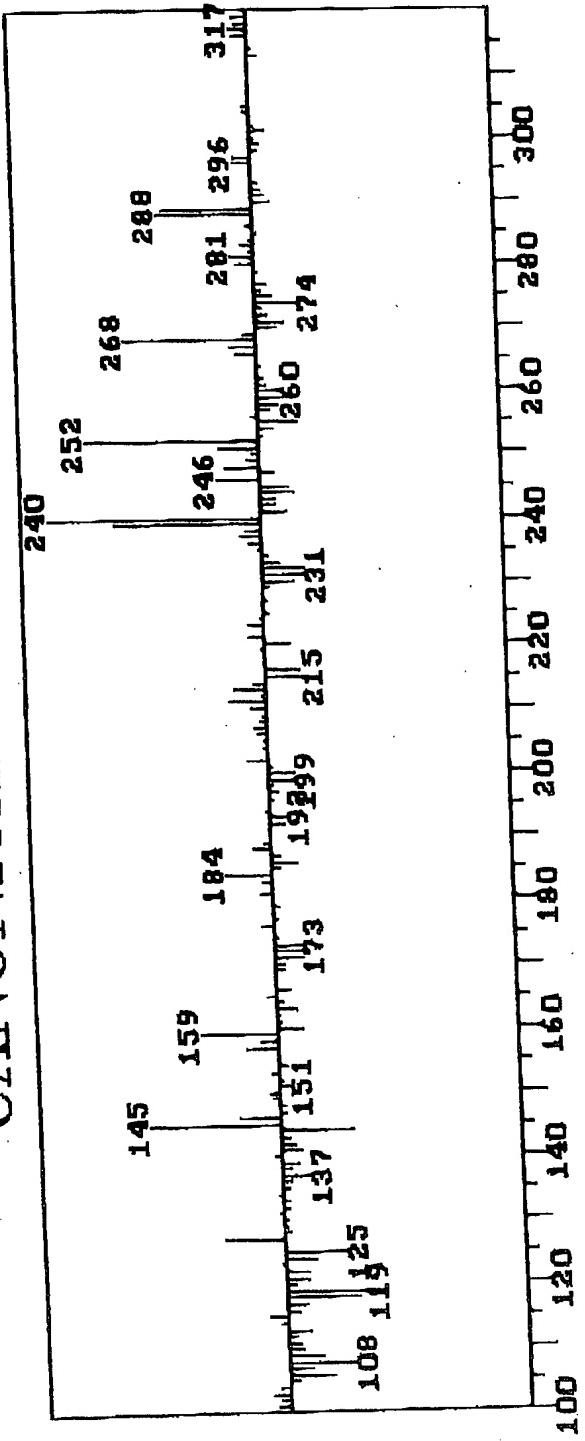
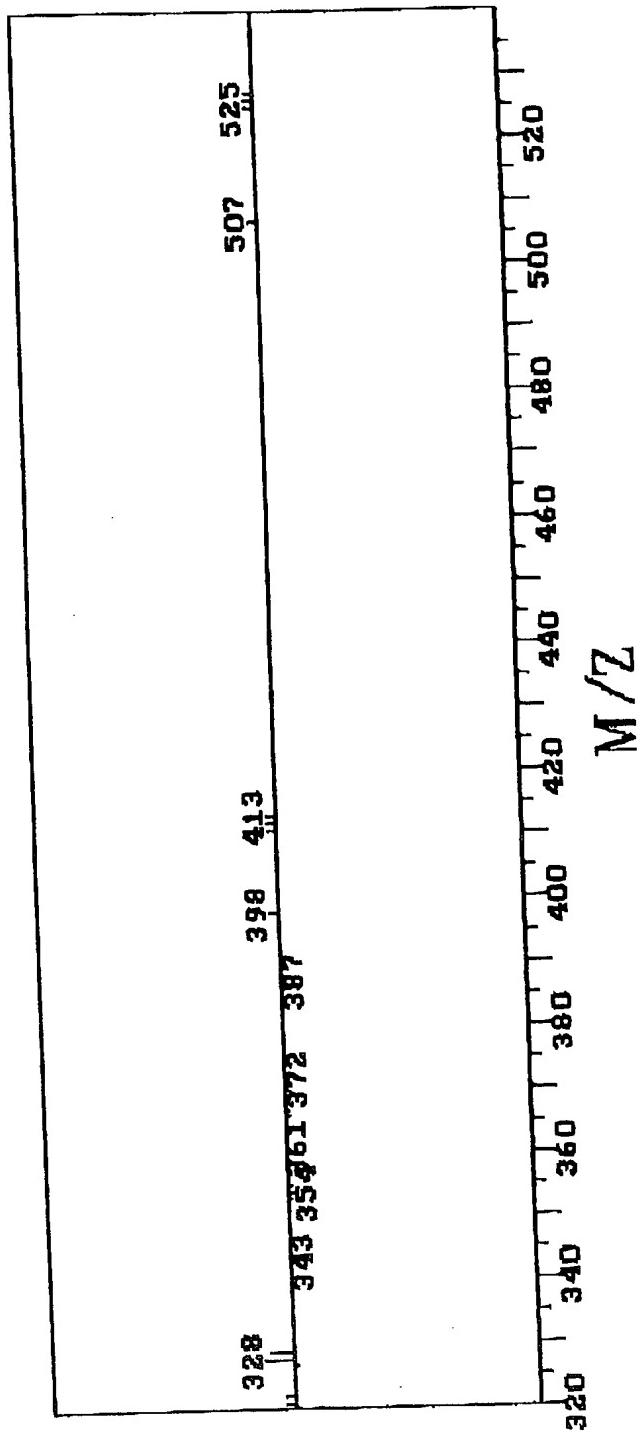


Fig 12(a)



CANONICAL VARIATE 1

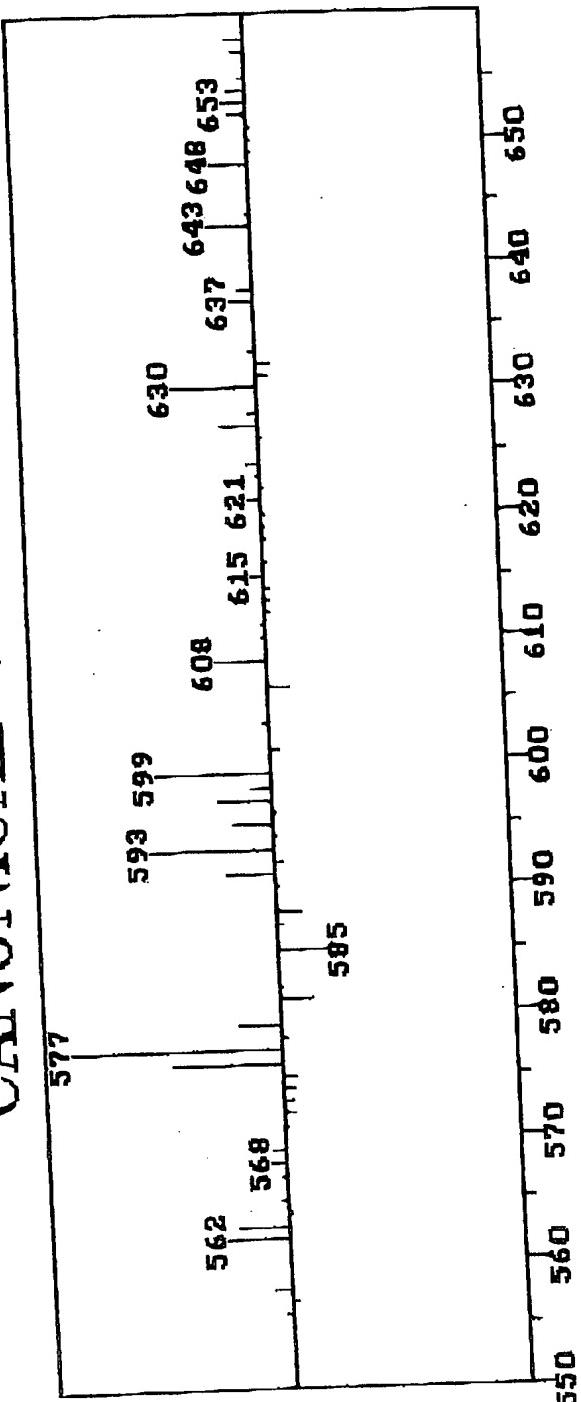
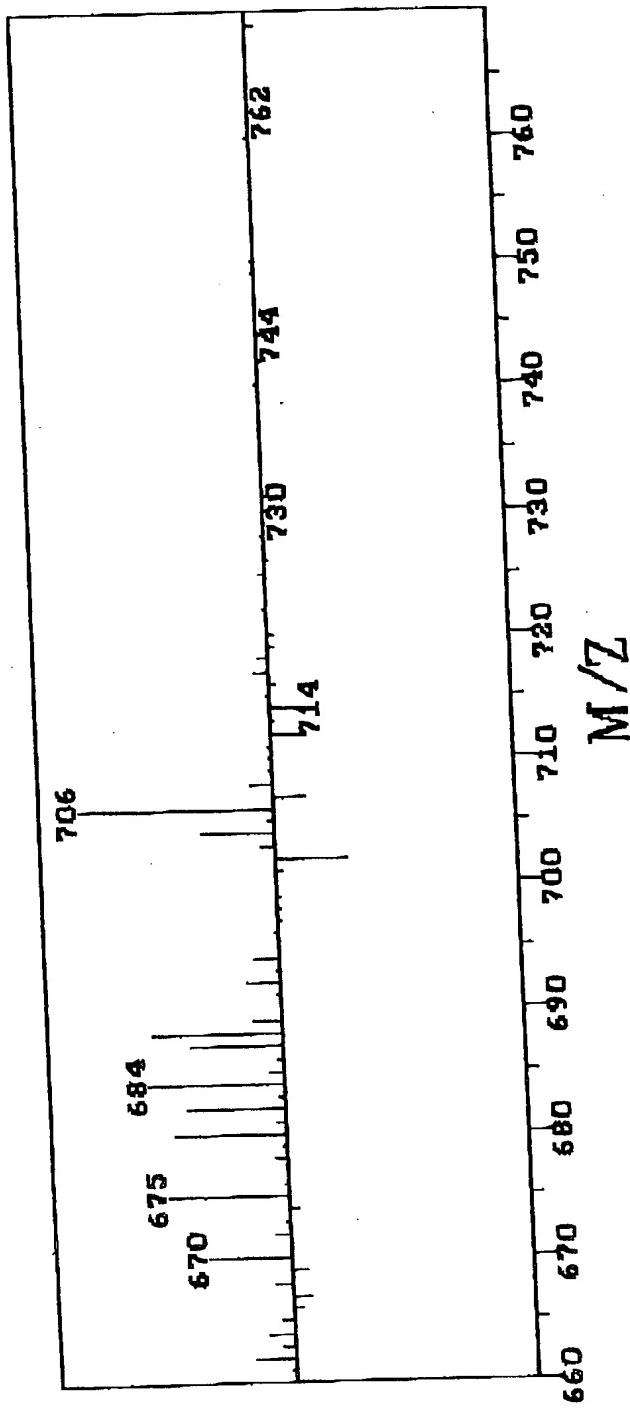


Fig 12(b)



M/Z

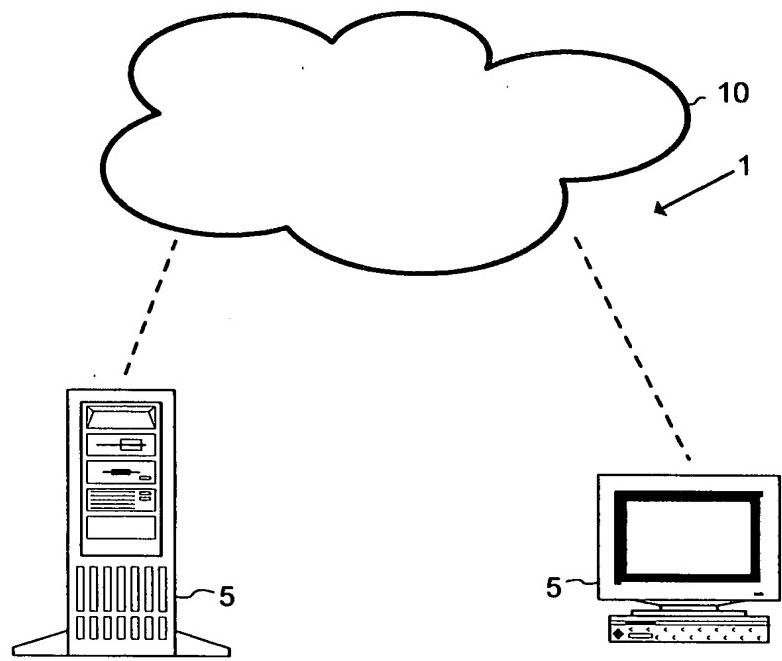


Fig 13

Fig. 14

